The stability and the shape of the heaviest nuclei

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In this paper, we report a systematic study of the heaviest nuclei within the relativistic mean field (RMF) model. By comparing our results with those of the Hartree-Fock-Bogoliubov method (HFB) and the finite range droplet model (FRDM), the stability and the shape of the heaviest nuclei are discussed. The theoretical predictions as well as the existing experimental data indicate that the experimentally synthesized superheavy nuclei are in between the fission stability line, the line connecting the nucleus with maximum binding energy per nucleon in each isotopic chain, and the β-stability line, the line connecting the nucleus with maximum binding energy per nucleon in each isobaric chain. It is shown that both the fission stability line and the β-stability line tend to be more proton rich in the superheavy region. Meanwhile, all the three theoretical models predict most synthesized superheavy nuclei to be deformed.

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I. INTRODUCTION

Recent claims of successful syntheses of superheavy elements 115 and 113 [1, 2] have aroused new enthusiasm about studies of superheavy nuclei in the nuclear physics community (see Refs. [3, 4, 5] and references therein). For a review of recent experimental progress of this subject, we refer the reader to Refs. [6, 7]. Conventional liquid drop models of finite nuclei forbid the existence of any nuclei with a proton number larger than 100, i.e. superheavy nuclei, due to the destructive Coulomb force. However, shell effects are found to be able to stabilize these nuclei, and therefore explain their very existences [8, 9]. It has long been predicted that there exist a large number of relatively long-lived superheavy nuclei, the so-called superheavy island, which is separated in neutron and proton numbers from the known heavy elements by a region of much higher instability. Although the experimentally-synthesized superheavy nuclei are indeed very heavy, it is generally believed that they are not examples of the originally sought island of superheavy elements.

On the theoretical side, a lot of efforts have been made to interpret the experimental results and make various predictions. A short review of the theoretical activities can be found in Ref. [5]. Nowadays, there are several categories of theoretical models often used to study superheavy nuclei: The first category is the liquid drop model and its many variants, such as the finite-range droplet model (FRDM) [10]; The second category is the non-relativistic Skyme-Hartree-Fock model; The third category is the relativistic mean field model. Using these models, fission barriers, alpha-decay energies, shell closures, single-particle spectra, and so on have been extensively discussed [5].

In recent years, the relativistic mean field model has received much attention due to its natural description of the spin-orbit interaction, the saturation properties of symmetric nuclear matter, and many other things that non-relativistic models have some difficulties to explain [11]. It has also been widely employed to study superheavy nuclei (a short review can be found in Ref.[5]). Due to the amount of computer resources needed, studies of superheavy nuclei in the relativistic mean field model have often been limited to either spherical assumption or a small part of the superheavy region. In this paper, we report the first systematic study of superheavy nuclei within the relativistic mean field model with the deformation effect and the pairing correlation properly treated. By comparing our RMF+BCS calculations with those of the Hartree-Fock-Bogoliubov (HFB) and finite range droplet model (FRDM), we hope to obtain some hints for the search of the superheavy island.

In particular, we would like to adress two interesting subjects: the stability and the shape of the heaviest nuclei. The stability of a superheavy nucleus is a very subtle subject. It is determined by many competing decay modes: alpha decay, spontaneous fission, beta decay, and etc. Except beta decay, the other two are very difficult to describe quantitively, which would involve complicated lifetime calculations. Beta decay, on the other hand, can be understood much more easily from the energy point of view, i.e. nuclei near the β-stability line are stable against beta decay. Similarly, a useful concept is the fission stability line, the line connecting the nucleus with maximum binding energy per nucleon in each isotopic chain, which is related to the minimum Q value of fission [12]. At this line, nuclei with fixed proton number have maximum binding energy per nucleon; therefore they would be stable against neutron emission, which can play an important role to synthesize superheavy nuclei at the first place [1, 2]. Hence, one would expect superheavy nuclei should not deviate too far from this line.

The shape of the heaviest nucleus can also influence its stability greatly [13]. The original island of superheavy elements is predicted to be around $Z = 114$ and $N = 184$

[14] mainly due to the fact that $_{184}114$ is predicted to be a doubly magic nucleus with spherical shape, where shell effect is the strongest. Recent investigations have provided somehow conflicting predictions for the next doubly magic system, for example, the non-relativistic forces SkM* and SkP seem to prefer $_{184}126$ instead of $_{184}114$ [15]. A more complete summary of various predictions of different models can be found in Ref. [5]. In this paper, we would like to compare our RMF+BCS predictions with those of the HFB model and the FRDM model in order to see whether a large number of spherical nuclei exist in these models, which would indicate the existence or nonexistence of the next doubly magic nucleus, or (less ambitiously) the next neutron (proton) shell closure.

This paper is organized as follows. In Section II, we briefly introduce the relativistic mean field model and explain the numerical details of our calculation. In Section III, the stabilities of superheavy nuclei are studied from the energy point of view. In Section IV, the shapes of superheavy nuclei predicted by different theoretical models are compared. The whole work is summarized in Section V.

II. THEORETICAL FRAMEWORK

In this section, we briefly describe the RMF+BCS calculations. The RMF+BCS calculations have been carried out using the model Lagrangian density with nonlinear terms for both σ and ω mesons as described in detail in Refs. [16, 17], which is given by

$$\begin{aligned}\mathcal{L} &= \bar{\psi}(i\gamma^{\mu}\partial_{\mu} - M)\psi \\ &+ \frac{1}{2}\partial_{\mu}\sigma\partial^{\mu}\sigma - \frac{1}{2}m_{\sigma}^{2}\sigma^{2} - \frac{1}{3}g_{2}\sigma^{3} - \frac{1}{4}g_{3}\sigma^{4} - g_{\sigma}\bar{\psi}\sigma\psi \\ &- \frac{1}{4}\Omega_{\mu\nu}\Omega^{\mu\nu} + \frac{1}{2}m_{\omega}^{2}\omega_{\mu}\omega^{\mu} + \frac{1}{4}g_{4}(\omega_{\mu}\omega^{\mu})^{2} - g_{\omega}\bar{\psi}\gamma^{\mu}\psi\omega_{\mu} \\ &- \frac{1}{4}R^{a}{}_{\mu\nu}R^{a\mu\nu} + \frac{1}{2}m_{\rho}^{2}\rho_{\mu}^{a}\rho^{a\mu} - g_{\rho}\bar{\psi}\gamma_{\mu}\tau^{a}\psi\rho^{\mu a} \\ &- \frac{1}{4}F_{\mu\nu}F^{\mu\nu} - e\bar{\psi}\gamma_{\mu}\frac{1-\tau_{3}}{2}A^{\mu}\psi,\end{aligned} \tag{1}$$

where all symbols have their usual meanings. The corresponding Dirac equation for nucleons and Klein-Gordon equations for mesons obtained with the mean-field approximation and the no-sea approximation are solved by the expansion method on the axially deformed harmonic-oscillator basis [18]. The number of shells used for expanding the nucleon and meson wave functions is chosen as $N_f = N_b = 20$. More shells have been tested for convergence considerations. Quadrupole constrained calculations [19] have been performed for all the nuclei considered here in order to obtain their energy surfaces and determine the corresponding ground-state deformations.

The pairing correlation plays an important role in studies of open-shell nuclei. It is also true for superheavy nuclei. In Ref. [3], it was shown that the use of a zero-range δ-force in the particle-particle channel can bring down the fission barrier compared to the use of a constant-gap pairing method. In the present calculation, the pairing correlation is treated by a state-dependent BCS method [20]. More specifically, the pairing force used is of the volume type

$$V = V_0\delta(\vec{r} - \vec{r}'). \tag{2}$$

In the past years, whether the pairing correlation in finite nuclei is of a volume type or surface type has been discussed a lot , but it seems that more investigations are still needed to reach a definite conclusion [21]; therefore, to limit the number of free parameters, we do not introduce explicitly any density dependence. On the other hand, to describe simultaneously both light and heavy nuclei [16], we introduce a weak mass number dependence to the pairing strength, i.e.

$$V_0 = 300 + 120/A^{1/3}, \tag{3}$$

which is purely phenomenological except for the $A^{1/3}$ dependence [22], For nuclei with an odd-number of nucleons, the blocking effect has been treated within the BCS framework [3, 9]. A more detailed description of the pairing method can be found in Ref. [3].

In the mean field channel, the effective force TMA [17] is used. The effective force TMA was first proposed to describe simultaneously both light and heavy nuclei. It in fact originated from two other very successful parameter sets: TM1 and TM2. TM1 aimed to describe the ground-state properties of heavy nuclei ($A > 40$) and TM2 those of light nuclei ($A < 40$). On the one hand, TMA inherited TM1's favorable property of being able to reproduce the essential feature of the equation of state and the vector and the scalar self-energies of the relativistic Bruckner-Hartree-Fock theory for nuclear matter [23]. On the other hand, it can also describe light nuclei very well. Its success comes from a weak mass dependence, which smoothly interpolates the TM1 and the TM2 parameter sets. We may interpret this mass dependence as a mean to effectively express the quantum fluctuations beyond the mean field level and/or the softness of the nuclear ground states in deformation, pairing and alpha clustering in light nuclei. Compared to other successful effective forces, such as NL3, the description of finite nuclei is of similar quality or slightly better [16], but TMA(TM1) yields a much softer equation of state at high density, which seems to be favored by current experimental results.

Finally, we would like to mention the strategy we used to confine our study to a reasonable number of nuclei since calculations of superheavy nuclei cost a lot of time. The number of nuclei is determined by including all of those compiled in Ref. [24] and extending the corresponding proton-rich limit and neutron-rich limit of a certain isotopic chain [24] by ten more nuclei, respectively (see also Fig.2). Using such a strategy, the number of superheavy nuclei investigated in the present study is around 600.

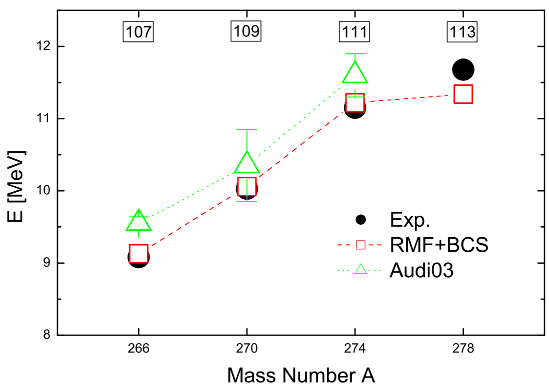

FIG. 1: (color online) α-decay energies of the $^{278}113$ α-decay chain. The latest experimental results of Morita et al. [2] are compared with the predictions of the RMF+BCS calculation and those compiled in Audi03 (obtained using "systematic trends") [24].

III. THE STABILITY OF SUPERHEAVY ELEMENTS

Before we study the stability of the heaviest nuclei, it is necessary to stress that although the parameters of the RMF+BCS model have not been constrained by any information from the superheavy region, the agreement of its predictions with existing experimental data is quite good in general, which has been demonstrated in the entire region (see Refs. [3, 5, 25, 26, 27] and references therein). Recently, Morita et al. has reported the synthesis of the new element 113 [2]. In Fig. 1, the experimental α-decay energies of the $^{278}113$ α-decay chain are compared with our predictions and those compiled in Audi03 (obtained using "systematic trends" [24]. It is clearly seen that the agreement is remarkable. A more detailed study is underway and will be reported somewhere else.

It was argued from the energy point of view that the fission stability line, the line connecting the nucleus with maximum binding energy per nucleon in each isotopic chain, plays an important role in studies of the stability of the heaviest nucleus in Ref. [12]. In Fig. 2 the binding energies per nucleon of the 600 nuclei we calculated are plotted as functions of the neutron number N (upper panel). The experimental data (lower panel) are taken from Ref. [24]. The nucleus with maximum binding energy per nucleon in each isotopic chain is denoted by a triangle. Those nuclei in different isotopic chains are then connected by dashed lines. It can be clearly seen that the area we investigated has in fact included the most bound nucleus in each isotopic chain. The theoretical curves are almost identical to the experimental ones (see also Fig. 3). Therefore, just as expected, all the experimental syntheses are indeed near the fission stability line [12]. Since the results of the HFB-8 [28] and FRDM [10] mass formulae are very similar to our calculations, they are not shown in this figure. Here, a few words about HFB-8 and FRDM are in place. The mass table of the finite-range droplet model has been around for more than ten years [10]. By carefully adjusting its parameters (about thirty) to the saturation properties of nuclear matter and the binding energies of around 1000 nuclei, it obtained a root-mean-square deviation of about 0.6 MeV for the binding energies of all the experimentally-known nuclei. HFB-8 is a rather new mass table based on the Hartree-Fock-Bogoliubov method [28]. By performing particle number projection, incorporating phenomenologically both the Wigner energy and the rotational energy, and meanwhile adjusting its parameters (around 20) to fit the saturation properties of nuclear matter and the binding energies of about 2000 nuclei, it achieved a similar quality to that of the FRDM model. More comparisons between these two models and current RMF models for nuclear ground-state properties can be found in Ref. [29].

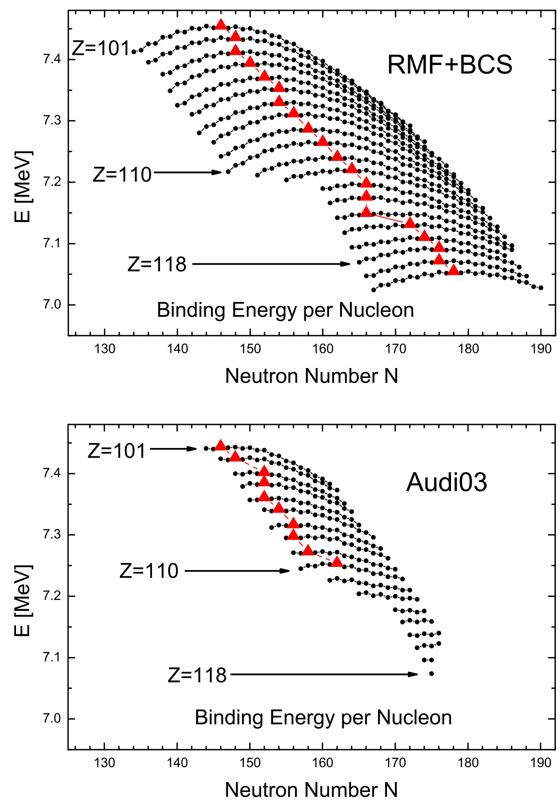

FIG. 2: (color online). Binding energies per nucleon of superheavy nuclei with $Z = 101$-120 and $N = 134$-190 as functions of the neutron number N. The theoretical predictions are compared with existing experimental data (including those obtained using "systematic trends") [24]. Different isotopes are connected by solid lines and ordered from top to bottom with increasing Z. The nucleus with maximum binding energy per nucleon in each isotopic chain is denoted by a triangle, and those of different isotopic chains are connected by dashed lines.

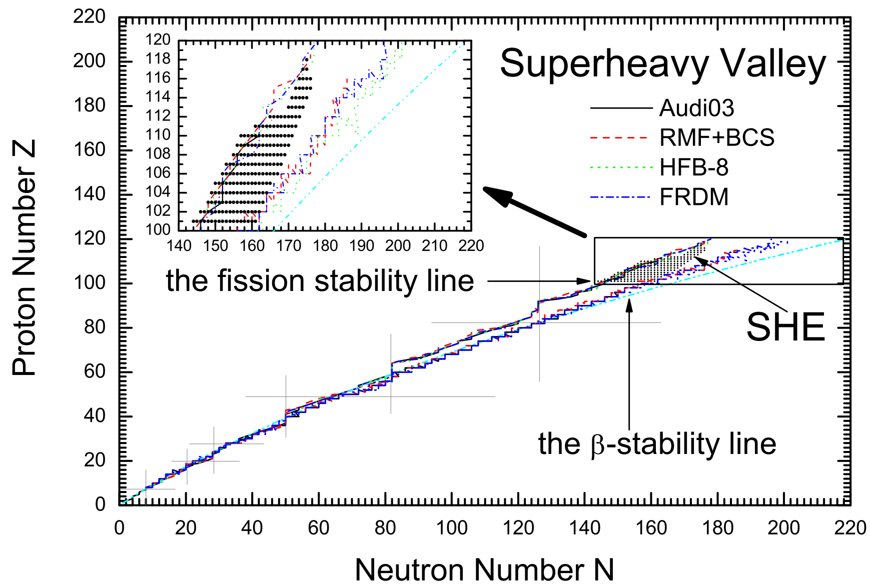

FIG. 3: (color online). The fission stability line and the β-stability line as functions of neutron number N and proton number Z. The theoretical predictions (RMF+BCS, HFB-8 [28] and FRDM [10]) are compared with existing experimental data (including those obtained using "systematic trends") [24]. The smooth dash-dot-dot line is the β-stability line of Bohr-Mottelson [13] (see text). The small black dots represent experimentally synthesized superheavy nuclei (SHE) (including those obtained using "systematic trends") [24].

In Fig. 3, the fission stability line and the β-stability line are plotted as functions of N and Z. The three theoretical predictions (RMF+BCS, HFB-8 [28] and FRDM [10]) are compared with existing experimental data [24]. For reference, the phenomenological β-stability line

$$N - Z = 6.0 \times 10^{-3} A^{5/3} \tag{4}$$

derived from the Bethe-Weizsäcker mass formula in Ref. [13] is also shown. Several interesting things can be learned immediately from Fig. 3. First, the microscopic (RMF+BCS, HFB-8 and FRDM) β-stability lines agree with each other very well, but they are bent up a little bit compared to the phenomenological β-stability line of Bohr-Mottelson. This difference can slightly change the definition of proton richness or neutron richness. As we can see from Fig. 3, superheavy nuclei have reached the β-stability line around $Z = 100$ if we use the microscopic β-stability lines. However, there is still a gap if we use the phenomenological β-stability line. In the following discussions, we will not distinguish the microscopic β-stability line and the phenomenological one. Second, all the three modern models predict quite similar most bound nuclei in each isotopic chain, which agree remarkably well with the experimental data. Third, the experimentally-synthesized superheavy nuclei populate to the left of the fission stability line and to the right of the β-stability line, the same as what we observed for those heavy nuclei with $89 \leq Z \leq 100$ [29]. This finding leads us to speculate that the center of the superheavy island is most probably in between these two lines. We will call this region the "superheavy valley". This speculation can find its support in "ordinary nuclei", where we know most nuclei exist along the β-stability line. But as we can see from Fig. 3, for them the fission stability line is quite close to the β-stability line. For heavier nuclei, such as actinide nuclei, they populate in between [29]. However, since we have not taken into account alpha-decay in this work, the exact location where the superheavy nucleus has the longest lifetime cannot be predicted. Lastly, the shell effects lead the most bound nucleus in each isotopic chain in the superheavy region to tend to have more protons, compared to their light- or medium-mass counterparts. The special role of neutron shell closure in this respect is most conspicuous at $N = 50$, 82 and 126. After three major neutron shell closures, the fission stability line deviates a lot from the β-stability line in the superheavy region, and thus, forms the so-called "superheavy valley".

The last observation above endows us with a powerful tool of identifying the next major neutron shell closure. That is to say there should also be a sudden increase in the fission stability line at the next major neutron shell closure. Using this argument, no neutron shell closure is found in the area we investigated, i.e. $N \leq 180$. It would be very interesting to study the $N > 180$ region, but it might be a difficult task due to the amount of computer resources needed. Fortunately, using our findings here, the searching region can be considerably reduced. Noticing that the fission stability line behaves as a linear function of N and Z between two major neutron shell

closures, we can approximate the theoretical and experimental fission stability lines (for $N > 126$) by the following formulae:

$$Z = (17.105 \pm 0.959) + (0.577 \pm 0.006)N \text{ (theory)}, \quad (5)$$
$$Z = 16.118 + 0.580N \text{ (Audi03)}. \quad (6)$$

The fission stability lines derived from the RMF+BCS, HFB-8 and FRDM calculations are all quite similar to each other, and therefore they have been averaged to obtain the above formula denoted by "theory". One should note that these approximations are valid only up to the next major neutron shell closure. Future investigations, therefore, can be performed along these lines with the fission stability line as the upper bound.

IV. SHAPES OF SUPERHEAVY NUCLEI

Most experimentally-synthesized superheavy nuclei are believed to be deformed. This could be verified from two aspects: First, studies of "ordinary nuclei" revealed that only magic nuclei are spherical; second, actinide nuclei are known to be strongly deformed. In Fig. 4, we plot the quadrupole deformation parameters, β_2, of the 600 nuclei we calculated as functions of neutron number N and proton number Z. It is quite interesting to note that both RMF+BCS and HFB-8 calculations predict very strongly prolate deformations, $\beta_2 \geq 0.45$, for those nuclei in the upper-right corner. Even for those nuclei in the lower-left corner, the deformation is still appreciable, with β_2 ranging from 0.15 to 0.35. However, there are two major differences between the predictions of the RMF+BCS calculations and those of the HFB-8 calculations. Firstly, there is a small number of spherical nuclei near $N = 184$ and $Z = 114$ in the HFB-8 calculations, but there is no spherical nucleus at all in the RMF+BCS calculations. Second, strongly prolate deformation occurs in the HFB-8 calculations at mass numbers smaller than those predicted by the RMF+BCS calculations; therefore it might indicate possible shape coexistence [3, 25, 30].

In other words, the RMF model with the effective force TMA predicts no doubly magic nucleus in the area we investigated. The HFB-8 calculations seem to prefer $^{298}_{184}114$ to be a doubly magic nucleus, but the deformation pattern predicted for these superheavy nuclei are different from those observed for "ordinary nuclei" [16, 29], where a much larger number of nuclei near the doubly magic nucleus are found to be spherical. Therefore a decisive conclusion is not possible. This is, in fact, consistent with the recent study of Ćwiok et al. [30], where they discussed the possibility of triaxial deformations for those nuclei near $N = 184$ and $Z = 114$. Thus, this difference is once again the old model dependence problem. In Ref. [5], the spherical doubly magic nuclei are searched for all the usual parameterizations while here TMA is used to investigate their deformations. One should note that the octupole deformation and other beyond mean-field correlations can greatly reduce the second fission barrier [31]; therefore, it would be interesting to investigate whether the conclusions of the present work would be modified if these correlations are taken into account.

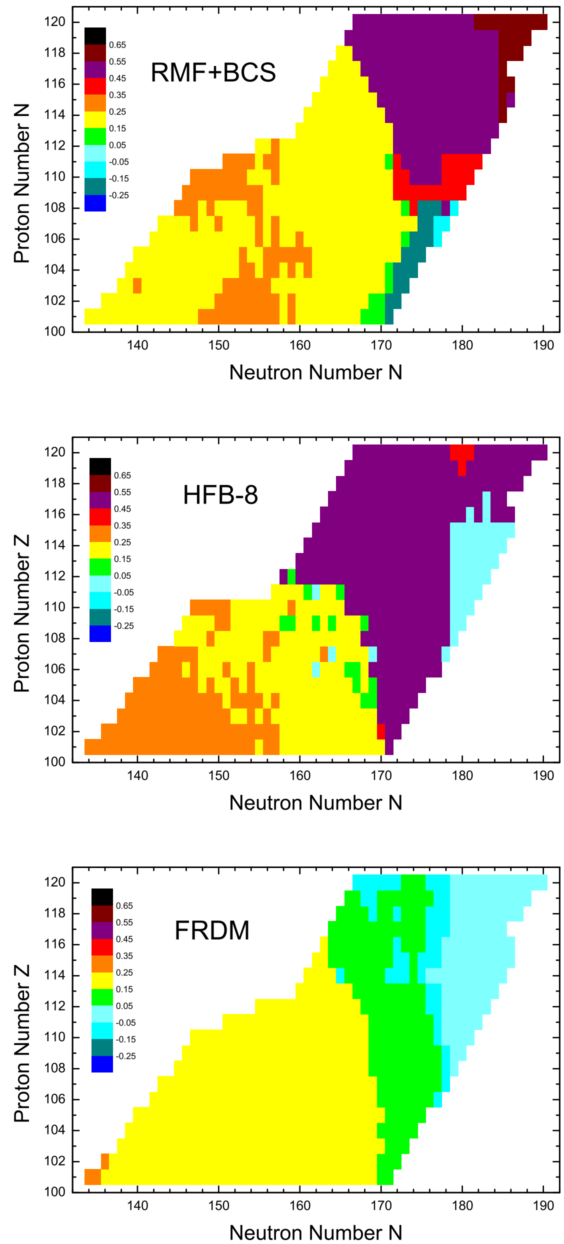

FIG. 4: (color online). Proton quadrupole deformation parameters, β_2, of superheavy nuclei with Z = 101-120 and N = 134-190 as functions of neutron number N and proton number Z. The predictions of the RMF+BCS calculations are compared with those of the HFB-8 [28] and FRDM [10] mass formulae.

It is to be noted that the most remarkable difference exists between the microscopic models, RMF+BCS and HFB-8, and the macroscopic-microscopic model, FRDM: FRDM displays a transition from moderately deformed shapes to spherical shapes from the lower-left corner to

the upper-right corner. That is to say we find a similar pattern that we observed for those conventional doubly magic nuclei [16, 29], i.e. spherical shapes for doubly magic nuclei and those nearby. Therefore once again we conclude that ${}^{298}_{184}114$ is probably a doubly magic nucleus in the FRDM calculations, or more precisely, there is probably a major shell closure at $N = 184$.

Of course, one should note that no clear indication of the $N = 184$ shell closure in the RMF+BCS and HFB-8 calculations (as shown in Fig.4) does not necessarily mean it does not exist. As well known nowadays, proton (neutron) shell closures are also neutron (proton) number dependent. Therefore, this implies if $N = 184$ is truly a neutron shell closure, we might have to look for the evidence in the region with $Z > 120$. Similarly, $Z = 114$ or $Z = 120$ might be a major proton shell closure in the more neutron rich side.

V. SUMMARY

By performing a RMF+BCS calculation of about 600 superheavy nuclei and employing the latest theoretical and experimental results, we have studied two extremely important subjects of superheavy nuclei, their stabilities and shapes. Both theory and experiment showed that all the experimentally-synthesized superheavy nuclei lie in between the fission stability line and the β-stability line, i.e. the "superheavy valley". It was also shown that the fission stability line and the β-stability line tend to be more proton rich than their light- or medium-mass counterparts. In this sense, it is justified to say that the observed "proton richness" of superheavy nuclei is not only a result of the limitation of current experimental methods but also a manifestation of their inherent nature. Although all the three theoretical models (RMF+BCS, HFB-8 and FRDM) predict most superheavy nuclei to be deformed, they differ from each other for those nuclei near $N = 184$. This model dependence might be removed by a more precise description of the single-particle spectra of the heaviest nuclei, which would be our next work.

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